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QUANTUM MECHANICAL CALCULATION OF CHARGE EXCHANGE
PROBABILITY DURING COLLISIONS

By

Yu. N. Demkov

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TRANSLATOR'S NOTE

The following two errors have been noticed in the Russian text of this paper:

Page 88 (of the Russian text): The first equation at the top of the page is missing the term following the multiplication sign.

Page 89 (of the Russian text): The last equation reads

$$w = \sin^2 \frac{1}{2h} \int_{-\infty}^{t^{\infty}} (E_{oa} - E_{os}) dt.$$

It should read

$$w = \sin^2 \frac{1}{2h} \int_{-\infty}^{+\infty} (E_{oa} - E_{os}) dt.$$

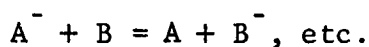
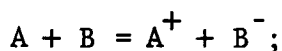
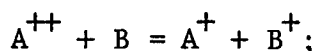
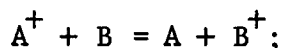
QUANTUM MECHANICAL CALCULATION OF CHARGE EXCHANGE PROBABILITY DURING COLLISIONS

By

Yu. N. Demkov

1. ESSENCE OF THE CHARGE EXCHANGE PROCESS

One of the possible results of a collision between two atomic systems (atoms, positive or negative ions) is a charge exchange, that is, a transfer of electrons from one system to another. These processes might be presented schematically by formulas in the same way as a nuclear reaction is presented. For instance:



Henceforth, all our examples will pertain to the first and second of these formulas, that is, to the collisions of positive ions with neutral atoms, since similar processes are of the highest practical interest.

Of particular interest is the case of the so-called resonance charge exchange, that is, a charge exchange during a collision of an atom and an ion of one and the same element. As was experimentally disclosed (Ref. 1), during the transition of ions through a gas the dispersion increases sharply if the gas is of the same nature as the ion (He^+ and He , H_2^+ and H_2 , etc.).

Therefore, large numbers of slow ions appear. This can be explained by the fact that the effective cross section of the resonance charge exchange is great. That is, the charge exchange can also take place at large impact parameters and the ion becomes transformed into a neutral atom while continuing to travel without deviations, and an atom becomes transformed into an ion and remains almost stationary.

Such an increase in the effective cross section of charge exchange, as will be shown further on, is connected with the fact that the electron in the given case does not change its energy during the transition /75

from one atom to another; that is, a unique resonance of the energy levels takes place. If on the other hand a similar resonance is absent, then the change in energy of the electron is compensated by a change in the kinetic energy of the nuclei. A similar energetic exchange hinders the process and decreases the effective cross section.

Strictly speaking a resonance charge exchange cannot be distinguished from an elastic scattering because the nuclei in this case are indistinguishable and, in the case of an accurate quantum mechanical calculation, it would be necessary to take into consideration a nuclear exchange. Considering that a neutral atom is unexcited before as well as after the collision, we would have then concluded that the scattering of ions occurs more frequently in the directions from $\theta \approx 0$ and $\theta \approx \pi$ (θ is the scattering angle of the ions motion from the original). The scattering of ions in the direction of $\theta \approx 0$ corresponds to an elastic collision, and a scattering in the direction of $\theta \approx \pi$ corresponds to a charge exchange. A nuclear exchange will basically have an effect on the scattering at intermediate angles, which takes place during close to head-on collisions. Such collisions are improbable and they do not influence the over-all results. Thus we might disregard a nuclear exchange, consider nuclei as being distinguishable and, by the same token, separate scattering and charge exchange.

Experimentally the problem is reduced to a calculation of the number of slow ions appearing during the passage through a gas of a beam of ions of the same gas.

Such experiments were conducted on numerous occasions (Ref. 2), whereby the following was discovered: an effective cross section of resonance charge exchange has a magnitude on the order of $100 a^2$ (a is the Bohr radius). This cross section decreases slowly with the increase of energy of the colliding particles; with the decrease of the ionization potential of the atom its effective cross section increases.

This paper presents a quantum mechanical calculation of charge exchange phenomena, whereby the above mentioned experimental results coincide with the results of our calculation.

The investigation of resonance charge exchange is necessary, particularly in order to explain the processes which take place in the plasma of a gaseous discharge, which consists of atoms and ions of any given element and electrons. A collision of all these particles takes place in the plasma at energies on the order of an electron volt.

It was pointed out for the first time by L. A. Sena (Ref. 3) that the resonance charge exchange plays a fundamental role among all phenomena that take place in plasma, since the cross section of charge exchange is large in comparison with the cross sections of other processes.

Therefore any given theory of a gas discharge plasma should /76 take into consideration the phenomena of charge exchange.

V. A. Fok based his work "On the Motion of Positive Ions in a Plasma" (Ref. 4), on the assumption of the fundamental role of charge exchange in a plasma. It is accepted in this paper that the cross section of charge exchange does not depend on the energy of the colliding particles, and the velocity distribution of ions is determined exclusively by a charge exchange.

All this makes the quantum mechanical calculation of a resonance charge exchange an urgent problem.

Among the methods which were applied during the examination of a charge exchange, the following can be mentioned:

1. The parametric method. In this method both nuclei are considered to be in the first approximation. The parametric method was applied for the first time for a charge exchange in the work by Brinkman and Kramers (Ref. 5). However, in the case of a resonance charge exchange their results are not good as far as it is known, since the first approximation in this case yields an untrue result for small impact parameters. On the other hand, in the case of an absence of a resonance, the result is true only at energies of more than 100 ev.

2. The Born approximation. This method is also applicable at energies of more than 100 ev. Calculations were conducted in the same paper by Brinkman and Kramers whereby the authors have discovered that the parametric method, as well as the Born approximation, leads to identical results. The reason for this was explained in the work by Mott (Ref. 6). It is proven in this paper that for large energies both methods are equivalent.

3. In addition, the phenomena of charge exchange were investigated by Massey and Smith (Ref. 7) using the method of distortion of wave functions. In their method the wave function is separated into specific functions of the electron in a field of two stationary nuclei. Such a method obviously is most accurate. However, the calculations are very cumbersome since wave functions are not accurately known and it is necessary to be satisfied with a very rough approximation; therefore, the result cannot be guaranteed. In the indicated work results were given only for the case of $\text{He}^+ + \text{He}$ at an ion energy of 1,000 ev.

4. Finally, a case of resonance charge exchange is discussed in particular in the book by L. A. Sena (Ref. 8). This author has achieved a very good agreement with experimental data; however, the results were

obtained in the presence of very loose assumptions so that these results pertain only to the qualitative evaluation of the phenomena.

This paper utilizes the parametric method. In the case of a resonance charge exchange this method is applied within very broad limits, beginning, for instance, with an energy of 1 ev and lower. This is /77 due to the fact that the relative speed of the nuclei does not change during collision.

In accordance with the proposition by P. P. Pavinsky, this method is somewhat changed so that it is applicable to a resonance charge exchange. In addition, within the framework of the parametric method one more general conclusion was investigated which makes it possible to obtain an angular distribution for a charge exchange and to substantiate the assumption of the first method as well as to present a point of fundamental interest.

2. THE PARAMETRIC METHOD

Both nuclei are considered to be two centers of force traveling along a determined trajectory; that is, a classical trajectory. The probability of charge exchange is calculated; that is, the transition of an electron from one nucleus to another during a collision. Calculations are made in the first approximation whereby the distinction from a common theory of distortion is contained in the selection of the function of zero approximation which already includes time implicitly as a result of the motion of the nuclei.

The forces of interaction between the neutral atom and the ion drop rapidly and the effect of charge exchange, as will be shown further on, in the case of a resonance of levels is already of considerable magnitude at large ranges. Therefore, it is possible to consider without gross error that, for instance, an ion in a given coordinate system de-excites when an atom travels past the ion at a prescribed distance D in uniform motion along a straight line with velocity v .

We will first of all examine a single electron problem. We will select such a system of coordinates in which the ion is located at the origin and the atom has the coordinates $(vt, D, 0)$; that is, the atom travels in uniform motion along a straight line. Then the problem is reduced to an investigation of the behavior of the electron in a field with a potential energy which depends on time. The Schroedinger equation will have the following form:

$$\left[-\frac{\hbar^2}{2m} \Delta + U_I(r) + U_A(r') \right] \Psi = i\hbar \frac{\partial \Psi}{\partial t}. \quad (2.1)$$

Here U_I and U_A are the potential energies of the electron in the field of the ion and atom, respectively;

$$r = \sqrt{x^2 + y^2 + z^2}; \quad r' = \sqrt{(x - vt)^2 + (y - D)^2 + z^2}.$$

Before the collision the electron is located near the atom in the fundamental state. This means that when $t = -\infty$, Ψ has the following form

$$\Psi = \psi_0(r') e^{\frac{i}{\hbar} mvx} e^{-\frac{i}{\hbar} (E_0 + \frac{mv^2}{2}) t}. \quad (2.2)$$

Here $\psi_0(r')$ satisfies the equation

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$$\left[-\frac{\hbar^2}{2m} \Delta' + U_A(r') \right] \psi_0(r') = E_0 \psi_0(r'). \quad (2.3)$$

The additional multiplier $e^{\frac{i}{\hbar} (mvx - \frac{mv^2}{2} t)}$ appears as a result of the progressive motion of the atom. In order to find the probability of capture of the electron by the ion during a collision, it is necessary to extend in time the wave function ψ up to $t \rightarrow +\infty$ and to separate it into functions of the final state:

$$\psi = \sum_n a_n(t) \phi_n(r) e^{-\frac{i}{\hbar} \epsilon_n t}. \quad (2.4)$$

Here ϕ_n are the wave functions of the electron in the field of the ion. These functions satisfy the equation

$$\left[-\frac{\hbar^2}{2m} \Delta + U_I(r) \right] \phi_n(r) = \epsilon_n \phi_n(r). \quad (2.5)$$

Then the probability of capture of the electron by the ion in an n - state will be

$$w_n = |a_n(+\infty)|^2. \quad (2.6)$$

In order to find a_n , we proceed as usual by substituting the expansion (2.4) in equation (2.1). We then have

$$\sum_n U_A(r') a_n(t) \phi_n(r) e^{-\frac{i}{\hbar} \epsilon_n t} = i\hbar \sum_n \dot{a}_n(t) \phi_n(r) e^{-\frac{i}{\hbar} \epsilon_n t}.$$

From this follows:

$$i\hbar \dot{a}_n = \int \phi_n^*(r) U_A(r') \psi d\tau \cdot e^{\frac{i}{\hbar} \epsilon_n t}. \quad (2.7)$$

It is obvious from the formulae (2.2) and (2.4) that all a_n , which pertain to the discrete spectrum when $t \rightarrow -\infty$, are approaching zero. From this follows:

$$i\hbar a_n(+\infty) = \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar} \epsilon_n t} dt \cdot \int \phi_n^* U_A \psi d\tau. \quad (2.8)$$

In this formula we may substitute the expression (2.2) for ψ , assuming in the zero approximation that the interaction between the atom and the ion is absent, and consequently the probability of charge exchange equals zero. Then the first approximation will be true only under 79 the condition that $w_n \ll 1$. By substitution we obtain

$$i\hbar a_n(+\infty) = \int e^{-\frac{i}{\hbar} (E_0 + \frac{mv^2}{2} - \epsilon_n) t} dt \int \phi_n^*(r) U_A(r') \psi_0(r') e^{\frac{i}{\hbar} mvx} d\tau. \quad (2.9)$$

We will investigate the simplest case of a collision between a proton and a hydrogen atom. We will calculate a_0 , which corresponds to a resonance charge exchange. Then

$$\phi_0(r) = \frac{1}{\sqrt{\pi a^3}} e^{-\frac{r}{a}}; \quad \psi_0(r') = \frac{1}{\sqrt{\pi a^3}} e^{-\frac{r'}{a}};$$

$$U_A = -\frac{e^2}{r}; \quad E_0 = \epsilon_0$$

and

$$i\hbar\dot{a}_0 = - \frac{e^2}{\pi a^3} \int e^{-\frac{1}{a}(r+r')} \cdot \frac{1}{r'} e^{\frac{i}{\hbar}mvx} \cdot d\tau \cdot e^{\frac{i}{\hbar}\frac{mv^2}{2}t}.$$

At energies of less than 100 ev on the part of the approaching atom the magnitude $\frac{mvx}{\hbar}$ becomes comparable to unity only in the case of such x at which the sub integral function is already small. Therefore, $e^{\frac{i}{\hbar}mvx}$ and $e^{\frac{i}{\hbar}\frac{mv^2}{2}t}$ may be considered as equaling one unit for these energies.

Then

$$i\hbar\dot{a}_0 = - \frac{e^2}{a} \left(1 + \frac{R}{a}\right) e^{-\frac{R}{a}}; R = \sqrt{(vt)^2 + D^2}.$$

Integrating by t from $-\infty$ to $+\infty$, we have:

$$i\hbar a_0(+\infty) = - \frac{e^2}{v} 2\rho \left[2K_1(\rho) + \rho K_0(\rho)\right]; \rho = \frac{D}{a}.$$

Thus, we have

$$w_0 = \left(\frac{e^2}{\hbar v}\right)^2 4\rho^2 \left[2K_1(\rho) + \rho K_0(\rho)\right]^2. \quad (2.10)$$

Here K_0 and K_1 are the Bessel functions of the hypothetical case. These functions are related to the Hankel functions of the first type.

$$K_0(\rho) = \frac{1}{2} \pi i H_0^{(1)}(i\rho); K_1(\rho) = -\frac{1}{2} \pi H_1^{(1)}(i\rho).$$

Curve I in Fig. 1 gives the dependence of $\lg w_0 + \lg E$ on the parameter of impact ρ . In order to directly obtain $\lg w_0$, it is necessary to use the line with the corresponding notation E on the right side as the abscissa axis. For instance

$$E = 100 \text{ ev}; \rho = 8.2; -\lg w_0 = -1; w_0 = 0.1.$$

The interrupted line which is presented is obtained if we use the asymptotic representation $\sqrt{\frac{\pi}{2\rho}} e^{-\rho}$ instead of $K_0(\rho)$ and $K_1(\rho)$. As can be seen from this graph, both curves coincide as far as $\rho > 2$ is concerned.

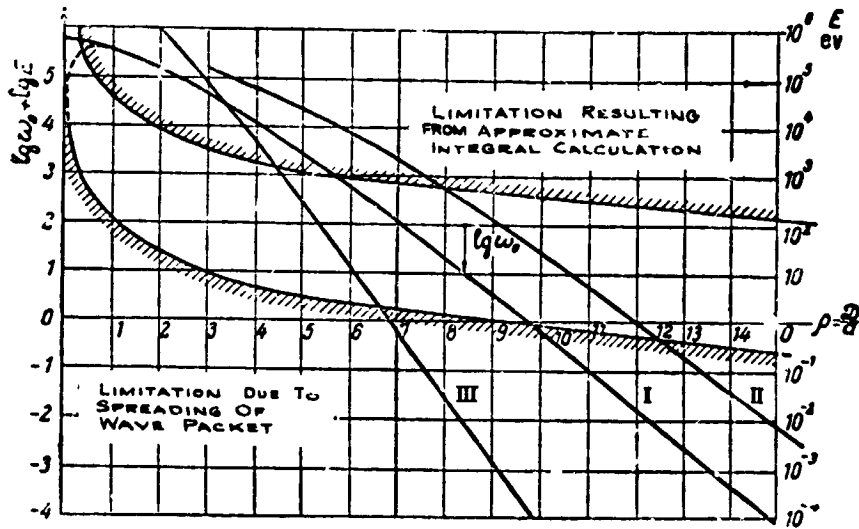


Fig. 1

Then

$$w_0 = \left(\frac{e^2}{h\nu}\right)^2 2\pi e^{-2\rho} \rho(\rho+2)^2. \quad (2.11)$$

As can be seen from this graph in the case of small ρ , w_0 is much larger than unity and obviously our approximation is not suitable. It is possible to assume (which will be proven further on), that the probability of a charge exchange in the case of these ρ varies between zero and unity and therefore such charge exchange probability may be considered to be on an average of $1/2$. Then the effective charge exchange area will be

$$\sigma \approx \frac{\pi \rho_0^2}{2}, \quad (2.12)$$

where ρ_0 is the value ρ , by which $w_0 = \frac{1}{2}$. The addition, which is due to the probability of a charge exchange when $\rho > \rho_0$, is insignificant

and consists of not more than 10% of the result, as can be easily proven. A more accurate expression is /81

$$\sigma \approx \frac{\pi}{2} \left(\rho_0 + \frac{1}{2} \right)^2. \quad (2.13)$$

Actually, in the case of $\rho > \rho_0$, we have

$$w_0 \approx A e^{-2\rho};$$

whereby

$$A e^{-2\rho_0} = \frac{1}{2}.$$

Then the addition to the effective cross section equals

$$\Delta\sigma = 2\pi A \int_{\rho_0}^{\infty} e^{-2\rho} \rho d\rho = 2\pi A \left(\frac{\rho_0}{2} + \frac{1}{4} \right) e^{-2\rho_0} = \pi \left(\frac{\rho_0}{2} + \frac{1}{4} \right)$$

and

$$\sigma \approx \frac{\pi \rho_0^2}{2} + \frac{\pi \rho_0}{2} + \frac{\pi}{4} \approx \frac{\pi}{2} \left(\rho_0 + \frac{1}{2} \right)^2.$$

However, the assumption in itself that $w_0 = \frac{1}{2}$ when $\rho < \rho_0$, is sufficiently rough so that a 10% error is also probable in the corrected formula.

The region which is shaded on the top (Fig. 1) corresponds to such values of ρ and E , for which $\frac{mva}{h} \rho > 1$, and therefore the multipliers $e^{\frac{i}{h} mvx}$ and $e^{-\frac{i}{h} \frac{mv^2}{2} t}$ should not be assumed to be equal to unity.

We will now examine within which limits we have the right to consider both nuclei as being classical particles. In accordance with the uncertainty principle, there should be present a certain inaccuracy in the determination of the coordinates and impulse of the nucleus. In addition, during the period of collision, a scattering of the wave packet will take place.

In order to have the right to treat the nucleus as a classical particle it is necessary that the inaccuracy in the determination of the coordinates should be much less than the parameter of the impact during the entire duration of the collision.

This period of time can be approximately evaluated as

$$\tau \sim \frac{2D}{v_x}.$$

Then, if the uncertainty of the coordinate was Δx before the collision, then after the collision it will equal

$$\Delta x' = \sqrt{(\Delta x)^2 + (\Delta v_x \tau)^2} \ll D;$$

From these two formulae follows the natural condition

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$$\Delta M v_x \ll M v_x$$

(M is the mass of the nucleus)

Finally, by utilizing the uncertainty principle it is easy to obtain

$$\rho \frac{M v a}{h} \gg 1. \quad (2.14)$$

The last inequality should be very strong because we square the strong inequality.

The area which is shaded on the bottom of the graph corresponds to the values E and ρ for which

$$\frac{M v a}{h} \rho < 100. \quad (2.15)$$

It is obvious that, in any case, beginning with an energy of 1 ev the theory is suitable.

We will mention that this is the principal range of application, contrary to the first range which is connected with the approximate calculation of the integral and cannot be expanded within the framework of a similar investigation.

The last assumption which we have made, to the effect that the distortion in the trajectory of the nuclei might be disregarded, is justified by the fact that the formulae are applied here for the case when $\rho \approx 10$. At such a distance for an atom with an energy of 1 ev

a deviation will be on the order of 1° , even if we take into consideration the polarizing forces.

We will also mention here that all these considerations are applicable, as can be easily proven, not only for hydrogen, but also in all other cases which are examined in this paper. Therefore, the area of applicability which is pointed out on the graph remains almost unchangeable for all three curves which are presented on it.

We will finally put down a clear expression for the effective cross section utilizing the fact that, within the range of applicability of the theory, it is possible to substitute the curve on the graph with a straight line with sufficient accuracy.

By disregarding the power factor it is possible to put down

$$Ew_0 = Ce^{-2\rho_0};$$

$$\frac{1}{2} E = Ce^{-2\rho_0};$$

$$\ln E = \ln 2C - 2\rho_0;$$

$$\sigma = \frac{\pi}{2} \left(A - \frac{1}{2} \ln E \right)^2.$$

By substituting $E = 1$ ev we find from the graph

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$$\sigma = \frac{\pi}{2} \left(10.5 - \frac{1}{2} \ln E \right)^2 \quad (2.16)$$

(E in this case is measured in ev; σ is measured, as always, in \AA^2).

Now let us examine a case when the resonance level is absent.

Then, integrating with respect to t , the oscillating multiplier $e^{\frac{1}{h}(\epsilon - E)t}$ in (2.9) strongly decreases the probability of a charge exchange.

For instance we will take the case of two nuclei with different charges $Z_a e$ and $Z_i e$. Let us assume that the nucleus with a charge $Z_a e$ had an electron in the 1S state before the collision.

Using the formula (2.9) we will calculate the probability of capture of an electron by a nucleus with a charge of $Z_i e$ also in its fundamental state. Then, in the formula (2.9), we will have

$$\phi_n = \phi_0 = \left(\frac{Z_i^3}{\pi a^3} \right)^{1/2} e^{-\frac{Z_i r}{a}}; \quad \psi_0 = \left(\frac{Z_a^3}{\pi a^3} \right)^{1/2} e^{-\frac{Z_a r}{a}};$$

$$U_A = -\frac{Z_a e^2}{r'}; \quad E_0 - \epsilon_0 = -\frac{e^2 Z_a^2}{2a} + \frac{e^2 Z_i^2}{2a} = \frac{e^2}{2a} (Z_i^2 - Z_a^2).$$

Integrating by $d\tau$, we will find

$$\begin{aligned} i\hbar \dot{a}_0 = & -\frac{8 e^2 (Z_a Z_i)^{5/2}}{a (Z_i^2 - Z_a^2)^2} \left[\frac{a}{R} \left(e^{-\frac{R}{a} Z_i} - e^{-\frac{R}{a} Z_a} \right) - \right. \\ & \left. - \frac{Z_i^2 - Z_a^2}{2Z_i} e^{-\frac{R}{a} Z_i} \right] e^{-\frac{i}{\hbar} \frac{e^2}{2a} (Z_i^2 - Z_a^2) t}. \end{aligned}$$

Integrating with respect to $t (R = \sqrt{(vt)^2 + D^2})$, we will find

$$w_0 = |a_0|^2|_{t=\infty} = 2^8 \frac{(Z_a Z_i)^5}{(Z_i^2 - Z_a^2)^4} \alpha^2 x$$

$$x \left[K_0 \left(A_a \frac{\rho}{2} \right) - K_0 \left(A_i \frac{\rho}{2} \right) - \frac{Z_i^2 - Z_a^2}{A_i} K_1 \left(A_{i2} \frac{\rho}{2} \right) \right]. \quad (2.17)$$

Here

$$\alpha = \frac{e^2}{\hbar v}; \quad \begin{aligned} A_a &= \sqrt{4z_a^2 + \alpha^2 (z_i^2 - z_a^2)^2}; \\ A_i &= \sqrt{4z_i^2 + \alpha^2 (z_i^2 - z_a^2)^2}. \end{aligned}$$

For instance, for the case when $z_a = 1$, $z_i = 2$ (the collision of a hydrogen atom with an α -particle)

$$\begin{aligned} w_0 &= \frac{2^{13}}{3^4} \alpha^2 \left[K_0 \left(\frac{\rho}{2} \sqrt{4 + 9\alpha^2} \right) - K_0 \left(\frac{\rho}{2} \sqrt{16 + 9\alpha^2} \right) - \right. \\ &\quad \left. - \frac{3}{\sqrt{16 + 9\alpha^2}} K_i \left(\frac{\rho}{2} \sqrt{16 + 9\alpha^2} \right) \right]. \end{aligned} \quad (2.18)$$

In the case when $E = 100$ ev, $w_0 = \frac{1}{2}$ already when $\rho \approx 0.04$.

However by using such a method only qualitative results can be obtained, because the assumption that the nucleus travels uniformly during the duration of the entire process is not true for the energies of the nuclei which are comparable in magnitude with the variation in their levels. A certain role is played here by the energetic exchange between the nuclei and the electrons, and this exchange cannot be fitted into the scheme of the parametric description.

A very interesting fact is that during the collision of a hydrogen atom with a α -particle a "random" resonance takes place between the 1s and 2s hydrogen levels of the 2p α -particle. We compute the probability of capture at the 2s-level. Then we will have in the formula (2.9)

$$\phi_n = \frac{1}{\sqrt{\pi a^3}} \left(1 - \frac{r}{a} \right) e^{-\frac{r}{a}}; \quad \psi_0 = \frac{1}{\sqrt{\pi a^3}} e^{-\frac{r'}{a}}; \quad U_A = -\frac{e^2}{r'}; \quad E_0 = \epsilon_n.$$

After integration we have:

$$i\hbar \dot{a}_2 = \frac{2e^2}{3a} \rho^2 e^{-\rho}; \quad \rho = \frac{R}{a} = \frac{1}{a} \sqrt{(vt)^2 + D^2}.$$

And after integrating with respect to t we have:

$$w_2 = \frac{16}{9} \alpha^2 \rho^2 \left[\rho K_0(\rho) + (2 + \rho^2) K_1(\rho) \right]^2. \quad (2.19)$$

The dependence $\lg w_2 + \lg E$ on ρ is presented in Fig. 1 by Curve II.

It is easy to prove that the probability of capture at the 2p-level equals zero in the first approximation.

By making the same conversions as previously, we obtain

$$\sigma = \frac{\pi}{2} \left(12.7 - \frac{1}{2} \ln E \right).$$

if we assume that the hydrogen atom de-excites, and E is the energy of the α -particle.

Thus, the electron should most frequently be captured at the excited level and then, with emission of the quanta ($\lambda \approx 300\text{\AA}$) or in the case of an inelastic impact of the second type, the electron should proceed to the ground state.

It is difficult to observe this effect experimentally because of the short wavelength of the emitted light and the difficulties in obtaining atomic hydrogen. However, it is probably impossible to select two such substances for which both these difficulties would not exist. The only necessity is that the difference between the levels should not be great.

Identifying the difference in levels by Δ , it is easy to obtain the condition of resonance from the formula (2.17): /85

$$\frac{e}{h\nu} \frac{2a}{e} \Delta < 1 \quad (2.20)$$

or approximately

$$\Delta < 0.1 \sqrt{\frac{E}{A}}.$$

Here E is the energy of the colliding particle, A is the atomic weight of the particles.

E and Δ are measured in electron volts.

3. THE ADIABATIC METHOD FOR CHARGE EXCHANGE CALCULATION

In the case of a resonance charge exchange another method can be applied which will yield results that will be valid within the same limits as before (in the unshaded part on our graph). However, this method will make it possible to eliminate the assumption that $w \ll 1$. By the same token we will have the opportunity to check the assumption on the behavior of $w(\rho)$ in the case when $\rho < \rho_0$.

We will assume that velocity of the atom is small and that, figuratively speaking, the electron will succeed in executing many turns along its orbit before the reciprocal position of the nuclei will undergo any noticeable change. That means that we will be able to consider, in null approximation, the nuclei at each moment as if they have relaxed. We will see that the expression for the probability of charge exchange will be obtained already at a null approximation. The first approximation and all other approximations which are obtained in a normal manner will not change the result and will allow us to become convinced of the proper selection of the null approximation.

We will examine the wave function of an electron which is located in the field of two identical nuclei which are at a considerable distance from each other. As before, the nucleus is considered to be classical. Then each energy level of a separate atom will correspond to two closed levels in the given system. In other words we have two solutions - a symmetrical and an antisymmetrical solution in regard to the coordinates of the nuclei.

We will define these solutions by

$$\Psi_{ns}(\vec{r}, \vec{R}, t); \Psi_{na}(\vec{r}, \vec{R}, t),$$

and the corresponding energies

$$E_{ns}(\vec{R}); E_{na}(\vec{R}).$$

Here \vec{r} is the radius vector of the electron;

\vec{R} is the radius vector of the relative position of the nuclei.

At sufficiently large R we can write

$$\begin{aligned}\Psi_{ns} &= \Psi_{ns}(\vec{r}, \vec{R}) e^{-\frac{i}{\hbar} E_{ns} t} = \frac{\Psi_{n1} + \Psi_{n2}}{\sqrt{2 + 2Q_n}} e^{-\frac{i}{\hbar} \left(E_n + \frac{A_n + B_n}{1 + Q_n} \right) t}; \\ \Psi_{na} &= \Psi_{na}(\vec{r}, \vec{R}) e^{-\frac{i}{\hbar} E_{na} t} = \frac{\Psi_{n1} - \Psi_{n2}}{\sqrt{2 - 2Q_n}} e^{-\frac{i}{\hbar} \left(E_n + \frac{A_n + B_n}{1 + Q_n} \right) t}.\end{aligned}\quad (3.1)$$

Here the following definitions are introduced:

A_n is the Coulomb integral of interaction,

B_n is the resonance integral of interaction,

Q_n is the superposition integral.

For these definitions we have the following expression

$$\begin{aligned}A_n(R) &= \int |\Psi_{n1}|^2 U_2 d\tau; \\ B_n(R) &= \int \Psi_{n1}^* U_1 \Psi_{n2} d\tau; \\ Q_n(R) &= \int \Psi_{n1}^* \Psi_{n2} d\tau,\end{aligned}$$

Ψ_{n1} and Ψ_{n2} are the specific functions of the n -state of the electron in the field of the first and second nuclei; U_1 and U_2 are the potential energies of the electron in the field of the first and the second nuclei, respectively.

The applicability of the formulae is determined by the smallness of Q_n in comparison with unity for large R -values, and therefore we might write approximately:

$$\begin{aligned}\Psi_{ns} &= \frac{1}{\sqrt{2}} (\Psi_{n1} + \Psi_{n2}); \quad \Psi_{na} = \frac{1}{\sqrt{2}} (\Psi_{n1} - \Psi_{n2}); \\ E_{ns} &= E_n + A_n + B_n; \quad E_{na} = E_n + A_n - B_n.\end{aligned}\quad (3.2)$$

Then the wave function will be:

$$\Psi_{ns} = \Psi_{ns} e^{-\frac{i}{h} E_{ns} t}; \quad \Psi_{na} = \Psi_{na} e^{-\frac{i}{h} E_{na} t}. \quad (3.3)$$

These functions, according to the original assumption, should be the approximate solution to the equation.

We should obviously consider that the force centers travel and that Ψ_{ns} , Ψ_{na} , E_{ns} and E_{na} depend implicitly on time by $\vec{R}(t)$. That is, for instance,

$$\Psi_{ns} = \Psi_{ns} [\vec{R}(t), \vec{r}] e^{-\frac{i}{h} E_{ns} [\vec{R}(t)]}.$$

However, in a wave function described in this manner, no consideration is given to its "pre-history". The value of the phase multiplier $e^{-\frac{i}{h} E(t) t}$ at the moment t_0 does not depend in this case on the form of the function $E(t)$ at all values of t ; it depends only on the value $E(t)$ at the moment t_0 . In fact the phase is an additive magnitude and is being "accumulated" during the entire duration of motion. Let us assume that the starting moment is $t = 0$ and we will find the phase at the moment t , taking into consideration this fact. For this purpose we will break up the time segment $(0, t)$ into small intervals: /87

$$t_0 = 0 < t_1 < t_2 \dots < t_n = t;$$

$$\Delta t_1, \Delta t_2, \dots \Delta t_n;$$

$$\Delta t_i = t_i - t_{i-1}.$$

The phase increase at each interval will be:

$$E(t_1)\Delta t_1, E(t_2)\Delta t_2, \dots, E(t_n)\Delta t_n$$

with an accuracy to the small numbers of the higher order.

Proceeding to the limit we will obtain the complete phase change

$$\int_0^t E(t) dt. \quad (3.4)$$

Thus, Ψ_{ns} and Ψ_{na} will be written as follows:

$$\Psi_{ns} = \Psi_{ns} e^{-\frac{i}{h} \int_0^t E_{ns} dt}; \quad \Psi_{na} = \Psi_{na} e^{-\frac{i}{h} \int_0^t E_{na} dt}. \quad (3.5)$$

In the presence of an \vec{R} , which does not depend on time, these functions pass on to (3.3).

We will mention that we have not as yet made any assumptions on the character of the relative motion of the nuclei.

The solution to the equation (2.1) will be sought in the following form

$$\Psi = \sum_n a_n(t) \Psi_{ns} e^{-\frac{i}{h} \int_0^t E_{ns} dt} + b_n(t) \Psi_{na} e^{-\frac{i}{h} \int_0^t E_{na} dt}. \quad (3.6)$$

By substitution in the equation we will obtain:

$$\begin{aligned} \sum_n \left[\dot{a}_n(t) \Psi_{ns} + a_n(t) \Psi_{ns} \right] e^{-\frac{i}{h} \int_0^t E_{ns} dt} + \\ + \left[\dot{b}_n(t) \Psi_{na} + b_n(t) \Psi_{na} \right] e^{-\frac{i}{h} \int_0^t E_{na} dt} = 0; \end{aligned}$$

$$\begin{aligned} \dot{a}_n + \sum_m a_m e^{-\frac{i}{h} \int_0^t (E_{ms} - E_{ns}) dt} \cdot \int \psi_{ns}^* \frac{d}{dt} \psi_{ms} d\tau + \\ + b_m e^{-\frac{i}{h} \int_0^t (E_{ma} - E_{ns}) dt} \cdot \int \psi_{ns}^* \frac{d}{dt} \psi_{ma} d\tau = 0 \end{aligned}$$

Considering that as a result of orthogonality and normalization,

$$\int \psi_n^* \frac{d}{dt} \psi_m d\tau = - \int \psi_m \frac{d}{dt} \psi_n^* d\tau ,$$

we have:

$$\begin{aligned} \dot{a}_n &= \int \psi_n \frac{d}{dt} \psi_{ns}^* d\tau \cdot e^{\frac{i}{h} \int_0^t E_{ns} dt} ; \\ b_n &= \int \psi_n \frac{d}{dt} \psi_{na}^* d\tau \cdot e^{\frac{i}{h} \int_0^t E_{na} dt} . \end{aligned} \quad (3.7)$$

Further on we obviously have to select Ψ in a null approximation and substitute in these formulae. In order to execute this, we will first examine the physical meaning of a_n , b_n at large distances between the nuclei.

Then

$$\begin{aligned} a_n(t) \psi_{ns} + b_n(t) \psi_{na} &= a_n(t) \frac{1}{\sqrt{2}} (\psi_{n1} + \psi_{n2}) e^{-\frac{i}{h} \int_0^t E_{ns} dt} + \\ &+ b_n(t) \frac{1}{\sqrt{2}} (\psi_{n1} - \psi_{n2}) e^{-\frac{i}{h} \int_0^t E_{na} dt} = \\ &= e^{-\frac{i}{h} \int_0^t E_{ns} dt} \left[\left(a_n + b_n e^{-\frac{i}{h} \int_0^t (E_{na} - E_{ns}) dt} \right) \psi_{n1} + \right. \\ &\quad \left. + \left(a_n - b_n e^{-\frac{i}{h} \int_0^t (E_{na} - E_{ns}) dt} \right) \psi_{n2} \right] . \end{aligned}$$

From this can be seen that the magnitude

$$w_n^{(1)}(t) = \frac{1}{2} \left| a_n(t) + b_n(t) \cdot e^{-\frac{i}{h} \int_0^t (E_{na} - E_{ns}) dt} \right|^2;$$

$$w_n^{(2)}(t) = \frac{1}{2} \left| a_n(t) - b_n(t) \cdot e^{-\frac{i}{h} \int_0^t (E_{na} - E_{ns}) dt} \right|^2 \quad (3.8)$$

The essence of the probability is to find an electron in an n-state [89] near the first or the second nuclei, respectively.

When $t \rightarrow -\infty$ (before the charge exchange), we obviously should put down $w_0^{(1)}(-\infty) = 1$, and all remaining $w_n = 0$. By defining

$$\frac{1}{h} \int_{-\infty}^0 (E_{na} - E_{ns}) dt = P \quad (3.9)$$

(P depends only on the form of the function $\vec{R}(t)$; that is, in the final calculation, on the parameter of the impact and the energy of the colliding particles.) We obtain from these conditions

$$a_n(-\infty) = b_n(-\infty) = 0 \quad n \neq 0; \quad a_0(-\infty) =$$

$$= \frac{1}{\sqrt{2}}, \quad b_0(-\infty) = \frac{1}{\sqrt{2}} e^{-iP}.$$

In a null approximation we will therefore have

$$\psi^{(0)} = \frac{1}{\sqrt{2}} (\psi_{0s} + \psi_{0a} \cdot e^{-iP}). \quad (3.10)$$

If we substitute this expression for ψ in the formula (3.7) and if we should make a very general assumption about the symmetry of the orbit of the nuclei (that is that $R(-t) = R(t)$), then it can be easily seen that $a_0(t)$, $b_0(t)$ will be antisymmetric time functions, and therefore

$$a_0(+\infty) = a_0(-\infty) = 1;$$

$$b_0(+\infty) = b_0(-\infty) = \frac{1}{\sqrt{2}} e^{-iP}.$$

By substituting these values in the formula (3.8) when $t \rightarrow +\infty$ and taking into consideration that in the case of an orbital symmetry, we have

$$\int_{-\infty}^0 (E_{0a} - E_{0s}) dt = \int_0^{\infty} (E_{0a} - E_{0s}) dt = P;$$

$$w_0^{(1)}(+\infty) = \frac{1}{4} |1 + e^{-2iP}| = \cos^2 P;$$

$$w_0^{(2)}(+\infty) = \frac{1}{4} |1 - e^{-2iP}| = \sin^2 P.$$

$w_0^{(2)}(+\infty)$, is obviously the probability of charge exchange and we have therefore in explicit form

$$w = \sin^2 \frac{1}{2h} \int_{-\infty}^{+\infty} (E_{0a} - E_{0s}) dt.$$

If we should assume that the distance between the nuclei /90 remains large, so that w is small, then it is possible to utilize the expression (3.2) in the case of E_{0a} and E_{0s} in the first approximation. Then we will obtain

$$\begin{aligned} w_0 &= \sin^2 \frac{1}{2h} \int_{-\infty}^{+\infty} [(E_0 + A - B) - (E_0 + A + B)] dt = \\ &= \sin^2 \frac{1}{h} \int_{-\infty}^{+\infty} B dt \approx \left[\frac{1}{h} \int_{-\infty}^{+\infty} \left(\int \Psi_{01} U_2 \Psi_{02} d\tau \right) dt \right]^2, \end{aligned} \quad (3.11)$$

which coincides with the expression (2.9) of Section 2 with an accuracy to values which we have already disregarded.

Thus, at large impact parameters we have obtained for w_0 the preceding expression and at small parameters, as was assumed in the beginning, we obtain a variation in the probability, ranging from zero to unity.

If the potential energy of interaction between an atom and an ion is known to us, then, considering that the particles travel along a classical trajectory, we easily obtain

$$w_0 = \sin^2 \sqrt{\frac{M}{2m}} \int_{R_0}^{\infty} \frac{(E_{aa} - E_{0s}) dR}{\sqrt{\left(1 - \frac{D^2}{R^2}\right) E - U(R)}} , \quad (3.12)$$

here: D is the impact parameter;

M is the given mass of the nucleus;

E is the energy of the nucleus;

R_0 is the largest root of the expression which is located under the radical.

All values should be considered as being in atomic units.

The values $E_{0a} - E_{0s}$ and U for various R are known, for instance in the case of H^+ , H (molecular ion of hydrogen), and thus it is possible to determine the correction for the trajectory distortion, as well as the angular distribution, if we consider that the classical expression for the inclination angle is

$$\theta = \pi - 2 \int_{R_0}^{\infty} \frac{\sqrt{E} D dR}{R^2 \sqrt{\left(1 - \frac{D^2}{R^2}\right) E - U(R)}} . \quad (3.13)$$

In order to evaluate the range of application of these formulae we will mention that the nuclei are treated as before as classical particles, and the earlier obtained evaluations remain valid. /91

In addition, there should obviously exist an evaluation which would limit the speed of motion of the nuclei, as was pointed out in the beginning of this section.

In order to conduct a relative evaluation we will mention that, in the case of a slowly changing potential from point to point, the coordinate part of the wave function might be presented as follows:

$$\frac{i}{\hbar} \int p dx$$

The condition of applicability of this semi-classical consideration will be, as is known

$$\frac{d\lambda}{dx} \ll 1, \text{ where } \lambda = \frac{\hbar}{p}.$$

Analogously we have also assumed here that the nuclei travel slowly; that is, the potential changes slowly in time and the time part of the wave function was presented as:

$$e^{-\frac{i}{\hbar} \int E dt}$$

The condition of applicability of such an assumption will be analogously

$$\frac{d\tau}{dt} \ll 1; \tau = \frac{\hbar}{E},$$

or

$$\hbar \frac{dE}{dt} \ll E^2, \text{ but } E \sim \frac{e^2}{a}, \frac{dR}{dt} \sim v.$$

From this

$$\hbar v \frac{dE}{dR} \ll \frac{e^4}{a^2}.$$

It is easy to prove that

$$\frac{dE}{dR} = f\left(\frac{R}{a}\right) \cdot \frac{e^2}{a^2},$$

where $f(\frac{R}{a})$ is the function which decreases exponentially with the increase of R and reaches a maximum on the order of 1 when $R \sim a$. Thus, we obtain

$$\frac{e^2}{\hbar v} \gg 1. \quad (3.14)$$

This limitation coincides with the limitation which appeared in our paper in the preceding section as a result of the approximate integral calculation.

Actually the multiplier $e^{\frac{i}{\hbar} m v x}$ appeared under the integral, /92 namely as a result of the motion of the nucleus. Here however we make an over-all examination of the wave functions of the electron in a field of relaxed nuclei, and we disregard the distortions which are introduced by their motion.

With this fact in particular is connected the result that in the first approximation we have obtained a zero probability of capture on the higher levels: by disregarding the distortions which are introduced by the motion of the nuclei we obtain a symmetrical problem relative to time, and the coefficients a_n, b_n will have identical values when $t = \pm \infty$ at any given approximation and not only the first.

We will also mention that we will disregard here the Van der Waal forces of polarization just as we did in the preceding chapter. However, as we have already seen, the charge exchange is determined by the separation of the levels $E_{0s} - E_{0a}$, and the Van der Waal forces have no noticeable effect on this separation since these are gravitational forces independent of the symmetry of state.

However, the effect of these forces should be evaluated during the determination of $U(r)$ in the formulae (3.12), (3.13).

For the sake of definition we have investigated here the collision between H^+ and H , however the formulae (3.10), (3.11), and (3.12) are also true for any other case because the form of the specific functions was not definitely corrected anywhere in the entire conclusion.

4. CHARGE EXCHANGE DURING THE COLLISION OF He^+ AND He

A three electron problem should be solved in this case.

The Schroedinger equation has the following form

$$\left[-\frac{\hbar^2}{2m} (\Delta_1 + \Delta_2 + \Delta_3) - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} - \frac{2e^2}{r_3} - \frac{2e^2}{r_1'} - \frac{2e^2}{r_2'} - \frac{2e^2}{r_3'} + \frac{e^2}{r_{12}} + \frac{e^2}{r_{13}} + \frac{e^2}{r_{23}} \right] \Psi = i\hbar \frac{d}{dt} \Psi. \quad (4.1)$$

The initial and final states of the system are presented schematically in Fig. 2.

We will disregard the exchange in the beginning and will consider that the electron e_2 transfers from one nucleus to another. Then the function of the initial state will be

$$\psi_0(\vec{r}_2' \vec{r}_3') \phi_0(\vec{r}_1) e^{\frac{i}{\hbar} m v (x_2 + x_3)} \cdot e^{-\frac{i}{\hbar} (E_m + \epsilon_n + m v^2) t}, \quad (4.2)$$

and the function of the final state, on which the expansion is conducted, will be

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$$\psi_m(\vec{r}_1 \vec{r}_2) \phi_n(\vec{r}_3') e^{\frac{i}{\hbar} m v x_3} \cdot e^{-\frac{i}{\hbar} (E_m + \epsilon_n + \frac{m v^2}{2}) t}. \quad (4.3)$$

In these expressions ψ_m and ϕ_n satisfy the equations:

$$\left[-\frac{\hbar^2}{2m} (\Delta_1 + \Delta_2) - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} + \frac{e^2}{r_{12}} \right] \psi_m(\vec{r}_1 \vec{r}_2) = E_m \psi_m(\vec{r}_1 \vec{r}_2); \quad (4.4)$$

$$\left[-\frac{\hbar^2}{2m} \Delta_3 - \frac{re^2}{r_3} \right] \phi_n(\vec{r}_3) = \epsilon_n \phi_n(\vec{r}_3). \quad (4.5)$$

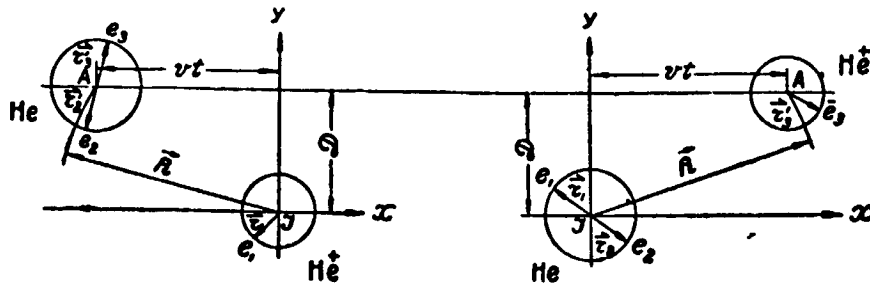


Fig. 2

The expansion of the unknown function Ψ according to the finite states will be

$$\Psi = \sum_{mn} a_{mn}(t) \Psi_m(\vec{r}_1, \vec{r}_2) \varphi_n(\vec{r}_3) e^{\frac{i}{\hbar} m v x_3} \cdot e^{-\frac{i}{\hbar} (E_m + \epsilon_n + \frac{m v^2}{2}) t} \quad (4.6)$$

Proceeding in the same manner, as in the case of hydrogen, we find by again disregarding the multipliers $e^{\frac{i}{\hbar} m v x}$ and $e^{-\frac{i}{\hbar} \frac{m v^2}{2} t}$ that

$$\begin{aligned} i \hbar \dot{a}_{mn}(t) &= e^2 \iiint \Psi_m^*(\vec{r}_1, \vec{r}_2) \varphi_n(\vec{r}_3') \times \\ &\times \left(-\frac{2}{r_3} - \frac{2}{r_1'} - \frac{2}{r_2'} + \frac{1}{r_{13}} + \frac{1}{r_{23}} \right) \Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3; t). \end{aligned} \quad (4.7)$$

By substituting (4.2) for Ψ in the null approximation, we obtain for the resonance charge exchange

$$\begin{aligned} i \hbar \dot{a}_{00} &= e^2 \iiint \Psi_0(\vec{r}_1, \vec{r}_2) \varphi_0(\vec{r}_3') \left(-\frac{2}{r_3} - \frac{2}{r_1'} - \frac{2}{r_2'} + \frac{1}{r_{13}} + \frac{1}{r_{23}} \right) \times \\ &\times \Psi_0(r_2' r_3') \varphi_0(r_1') d\tau_1 d\tau_2 d\tau_3 = e^2 (I_1 + I_2 + I_3 + I_4 + I_5). \end{aligned} \quad (4.8)$$

The function φ_0 is accurately known:

$$\varphi_0 = \left(\frac{8}{\pi a^3} \right)^{1/2} e^{-\frac{2r_3}{a}}.$$

A good approximation for the function Ψ_0 is the expression

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$$\Psi_0 = \left(\frac{z^3}{\pi a^3} \right)^{1/2} e^{-\frac{z}{a} (r_1 + r_2)}, \quad z = 2 - \frac{5}{16} = \frac{27}{16}.$$

If we would substitute these expressions in the formula (4.8), then the integrals could be calculated to the end. For this purpose it is necessary to transfer to elliptical coordinates.

We will obtain

$$\begin{aligned}
 I_1 = I_2 &= -\frac{1}{a} \frac{2^{10} \cdot z^3}{(z+2)^6} \left(1 + zp + \frac{1}{3} z^2 p^2\right) \times \\
 &\times \left[\frac{1}{p} e^{-zp} - \left(\frac{1}{p} + \frac{z+2}{2} \right) e^{-2(z+1)p} \right]; \\
 I_3 &= -\frac{1}{a} \frac{2^{10} \cdot z^4}{(z+2)^6} \left(1 + zp + \frac{1}{3} z^2 p^2\right) e^{-zp}; \\
 I_4 &= \frac{1}{a} \frac{2^9 \cdot z^3}{(z+2)^6} \left\{ \frac{1}{p} e^{-zp} - \left[\frac{1}{p} + \frac{11}{16} (z+2) + \frac{3}{16} (z+2)^2 p + \right. \right. \\
 &\left. \left. + \frac{1}{48} (z+2)^3 p^2 \right] e^{-2(z+1)p} \right\} \left(1 + zp + \frac{1}{3} z^2 p^2\right); \quad (4.9) \\
 I_5 &= \frac{1}{a} \cdot \frac{2^9 z^4}{(z+2)^6} \left\{ (1 + zp) e^{-zp} - \frac{4z^3}{(3z+2)(z+2)^2} \left[\frac{(z+2)(5z+4)}{z} - \right. \right. \\
 &\left. \left. - \frac{2(7z+6)}{3z+2} \cdot \frac{1}{p} \right] e^{-zp} + \left(z+2 + \frac{2(7z+6)}{3z+2} \frac{1}{p} \right) e^{-2(z+1)p} \right\}; \\
 p &= \frac{1}{a} \sqrt{(vt)^2 + D^2}.
 \end{aligned}$$

After integration with respect to t we have

$$\begin{aligned}
 iha_0(+\infty) &= \frac{2e^2}{v} \left\{ (-1.35 - 5.57 \rho^2) K_0(z\rho) - 18.89 \rho K_1(z\rho) + \right. \\
 &\quad + (1.35 + 7.70 \rho^2 - 4.45 \rho^4) K_0[2(z+1)\rho] + \\
 &\quad \left. + (12.01 \rho - 2.50 \rho^3 - 0.97 \rho^5) K_1[2(z+1)\rho] \right\}. \quad (4.10)
 \end{aligned}$$

The part containing $K_0 \left[2(z+1)\rho \right]$ and $K_1 \left[r(z+1)\rho \right]$ when $\rho > 3$ in this expression is negligibly small in comparison with the first part due to the rapid decrease of these functions, and therefore it may be disregarded. Then, by substituting once more the asymptotic presentation of the function $K_0(z\rho)$ and $K_1(z\rho)$, we have

$$w = \alpha^2 \pi \frac{1}{z\rho} (5.57 \rho^2 + 18.89 \rho + 1.35)^2 e^{-2z\rho}. \quad (4.11)$$

If we should carry out these simplifications, then we would also obtain in the preceding formulae

$$w = \frac{\pi}{2} \left(7.0 - \frac{1}{2z} \ln E \right)^2. \quad (4.12)$$

Curve III in Fig. 1 represents the dependence of $\lg w_0 + \lg E$ on ρ for that case. /95

Let us see now how our results will change if we take into consideration the property of symmetry of the wave function.

In order to obtain correct functions by which the decomposition is conducted, the functions (4.3) should be anti-symmetrized, for instance, along the coordinates \vec{r}_1, \vec{r}_3 . Then

$$\begin{aligned} \Psi = \sum_{mn} a_{mn}(t) \frac{1}{\sqrt{2}} \left[\Psi_m(\vec{r}_1, \vec{r}_2) \varphi_n(\vec{r}_3) - \right. \\ \left. - \Psi_m(\vec{r}_2, \vec{r}_3) \varphi_n(\vec{r}_1) \right] e^{-\frac{i}{h}(E_m + \epsilon_n)t}, \end{aligned} \quad (4.13)$$

if we assume, as we did everywhere, that the multiplier $e^{\frac{i}{h}mvx}$ and $e^{-\frac{i}{h}mv^2 \frac{t}{2}}$ equal a unit.

It should be mentioned that the properties of orthogonality and normality are not carried out properly for the functions along which the decomposition is conducted. However, we will always assume that these properties are accurate by disregarding the higher degrees of the superposed integrals which appear during a strict examination. Since we are

interested only in collisions with large impact parameters, this assumption does not impair our results.

It is also necessary to symmetrize the null approximation. According to the adopted scheme, it is necessary first of all to symmetrize $\Psi^{(0)}$ by \vec{r}_1, \vec{r}_2 and then we must anti-symmetrize by \vec{r}_1, \vec{r}_3 :

$$\begin{aligned} \Psi^{(0)} &= c \left[\psi_0(\vec{r}_2', \vec{r}_3') \varnothing_0(\vec{r}_1) + \psi_0(\vec{r}_1', \vec{r}_3') \varnothing_0(\vec{r}_2) - \right. \\ &\quad \left. - \psi_0(\vec{r}_1', \vec{r}_2') \varnothing_0(\vec{r}_2) - \psi_0(\vec{r}_1', \vec{r}_3') \varnothing_0(\vec{r}_2) \right] e^{-\frac{i}{\hbar}(E_0 + \epsilon_0)t} = \\ &= \frac{1}{\sqrt{2}} \left[\psi_0(\vec{r}_1', \vec{r}_3') \varnothing_0(\vec{r}_1) - \psi_0(\vec{r}_1', \vec{r}_2') \varnothing_0(\vec{r}_3) \right] e^{-\frac{i}{\hbar}(E_0 + \epsilon_0)t}. \quad (4.14) \end{aligned}$$

Further on we do the same as in the preceding case with certain complications.

By substituting the resolution Ψ in the equation (4.1), we obtain

$$\begin{aligned} \sum_{mn} i\hbar \dot{a}_{mn}(t) \left[\psi_m(\vec{r}_1, \vec{r}_2) \varnothing_n(\vec{r}_3') - \psi_m(\vec{r}_2, \vec{r}_3) \varnothing_n(\vec{r}_1') \right] e^{-\frac{i}{\hbar}(E_m + \epsilon_n)t} = \\ = \sum_{mn} e^2 \left\{ \left[-\frac{2}{r_3} - \frac{2}{r_1'} - \frac{2}{r_2'} + \frac{1}{r_{13}} + \frac{1}{r_{23}} \right] \psi_m(\vec{r}_1, \vec{r}_2) \varnothing_n(\vec{r}_3') - \right. \\ \left. - \left[-\frac{2}{r_3} - \frac{2}{r_2'} - \frac{2}{r_3'} + \frac{1}{r_{12}} + \frac{1}{r_{13}} \right] \psi_m(\vec{r}_2, \vec{r}_3) \varnothing_n(\vec{r}_1') \right\} e^{-\frac{i}{\hbar}(E_m + \epsilon_n)t}. \quad (4.15) \end{aligned}$$

Considering the functions by which the resolution is conducted as being orthogonal, as was previously stated, we have

$$\begin{aligned}
2i\hbar\dot{a}_{00} = & e^2 \iiint \left[\psi_0^* (\vec{r}_1, \vec{r}_2) \phi_0^* (\vec{r}_3') - \psi_0^* (\vec{r}_2, \vec{r}_3) \phi_0^* (\vec{r}_1') \right] \times \\
& \times \left[\left(-\frac{2}{r_3} - \frac{2}{r_1'} - \frac{2}{r_2'} + \frac{1}{r_{13}} + \frac{1}{r_{23}} \right) \sum_{mn} a_{mn} \psi_m (\vec{r}_1, \vec{r}_2) \phi_n (\vec{r}_3') - \right. \\
& \left. - \left(-\frac{2}{r_1} - \frac{2}{r_2'} - \frac{2}{r_3'} + \frac{1}{r_{12}} + \frac{1}{r_{23}} \right) \sum_{mn} a_{mn} \psi_m (\vec{r}_2, \vec{r}_3) \phi_n (\vec{r}_1') \right] d\tau_1 d\tau_2 d\tau_3.
\end{aligned} \tag{4.16}$$

Now it is necessary to see which sums (located after each of the parentheses) pertain to which parts of the function $\Psi^{(0)}$.

For this purpose we will resolve $\Psi^{(0)}$ by the final states

$$\begin{aligned}
\Psi^{(0)} = & \left[\psi_0 (\vec{r}_2', \vec{r}_3') \phi_0 (\vec{r}_1) - \psi_0 (\vec{r}_1, \vec{r}_2') \phi_0 (\vec{r}_3) \right] e^{-\frac{i}{\hbar} (E_0 + \epsilon_0) t} = \\
= & \sum_{mn} a_{mn}^{(0)} \left[\psi_m (\vec{r}_1, \vec{r}_2) \phi_n (\vec{r}_3') - \psi_m (\vec{r}_2, \vec{r}_3) \phi_n (\vec{r}_1') \right] e^{-\frac{i}{\hbar} (E_m + \epsilon_n) t},
\end{aligned}$$

where from

$$\begin{aligned}
a_{mn}^{(0)} = & \iiint \left[\psi_m^* (\vec{r}_1, \vec{r}_2) \phi_n^* (\vec{r}_3') - \psi_m^* (\vec{r}_2, \vec{r}_3) \phi_n^* (\vec{r}_1') \right] \times \\
& \times \left[\psi_0 (\vec{r}_2', \vec{r}_3') \phi_0 (\vec{r}_1) - \psi_0 (\vec{r}_1, \vec{r}_2') \phi_0 (\vec{r}_3) \right] \times \\
& \times d\tau_1 d\tau_2 d\tau_3 \cdot e^{-\frac{i}{\hbar} (E_0 + \epsilon_0 - E_m - \epsilon_n) t}.
\end{aligned} \tag{4.17}$$

The products which are located opposite are proportional to the cube of the transposition integral, and the two other products are proportional to its first power. By disregarding the first we obtain

$$\begin{aligned}
& \sum_{m n} a_{mn}^{(0)} \psi_m (\vec{r}_1, \vec{r}_2) \varphi_n (\vec{r}_3') \cdot e^{-\frac{i}{\hbar} (E_m + \epsilon_n) t} = \\
& = \psi_0 (\vec{r}_2', \vec{r}_3') \varphi_0 (\vec{r}_1) \cdot e^{-\frac{i}{\hbar} (E_0 + \epsilon_0) t}; \\
& \sum_{m n} a_{mn}^{(0)} \psi_m (\vec{r}_2, \vec{r}_3) \varphi_n (\vec{r}_1') \cdot e^{-\frac{i}{\hbar} (E_m + \epsilon_n) t} = \\
& = \psi_0 (\vec{r}_1', \vec{r}_2') \varphi_0 (\vec{r}_3) e^{-\frac{i}{\hbar} (E_0 + \epsilon_0) t}.
\end{aligned} \tag{4.18}$$

Thus

$$\begin{aligned}
2i\hbar\dot{a}_{00} &= e^2 \iiint [\psi_0^* (\vec{r}_1, \vec{r}_2) \varphi_0^* (\vec{r}_3') - \psi_0^* (\vec{r}_2, \vec{r}_3) \varphi_0^* (\vec{r}_1')] \times \\
&\times \left[\left(-\frac{2}{r_3} - \frac{2}{r_1'} - \frac{2}{r_2'} + \frac{1}{r_{13}} + \frac{1}{r_{23}} \right) \psi_0 (\vec{r}_2', \vec{r}_3') \varphi_0 (\vec{r}_1) - \right. \\
&\left. - \left(-\frac{2}{r_1} - \frac{2}{r_2'} - \frac{2}{r_3'} + \frac{1}{r_{12}} + \frac{1}{r_{13}} \right) \psi_0 (\vec{r}_1, \vec{r}_2') \varphi_0 (\vec{r}_3) \right] d\tau_1 d\tau_2 d\tau_3. \tag{4.19}
\end{aligned}$$

Schematically the right part has the following form

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$$\left[A (1, 2, 3) - A (3, 2, 1) \right] \cdot \left[B (1, 2, 3) - B (3, 2, 1) \right].$$

Both products 1-1 and 2-2 are equal; also equal are the products 1-2 and 2-1.

We have therefore

$$i\hbar\dot{a}_{00} = f - g. \tag{4.20}$$

Here: f is the integral (4.7), which was already calculated;
 g is the correction which was obtained as a result of the exchange consideration.

$$g = e^2 \iiint \psi_0(\vec{r}_1, \vec{r}_2) \phi_0(\vec{r}_3) \left[-\frac{2}{r_1} - \frac{2}{r_2} - \frac{2}{r_3} + \frac{1}{r_{12}} + \frac{1}{r_{13}} \right] \times$$

$$\times \psi_0(\vec{r}_1', \vec{r}_2') \phi_0(\vec{r}_3) d\tau_1 d\tau_2 d\tau_3 = e^2 [k_1 + k_2 + k_3 + k_4 + k_5]. \quad (4.21)$$

By substituting the values ψ_0 and ϕ_0 we could have calculated the integrals K_i ; however, it is obvious that all of them will be indirectly decreasing with the increase of R , since $e^{-2(z+1)\frac{R}{A}}$, and will therefore introduce a correction only to that part of the integral, f , which we have already disregarded. Thus, the electron exchange plays no role during the charge exchange, since this effect is already considerable at large impact parameters.

5. THE CASE OF ARBITRARY ATOMS

For the calculation of resonance charge exchange we can again utilize the fact that the probability of the process is great during large parameters of impact, and therefore the fundamental role in the formulae is played by the behavior of the wave function of the electron at large distances from the nucleus. Therefore, we may consider approximately that

$$\psi_0 = Ce^{-\frac{r}{h}\sqrt{2mU_i}} \quad (5.1)$$

or

$$\psi_0 = \sqrt{\frac{z^3}{\pi a^3}} e^{-\frac{z}{a}r}, \quad (5.2)$$

where

$$z^2 = \frac{U_i}{13.5},$$

U_i is, in this case, the ionization potential expressed in electron volts.

In addition the function $U_A(\vec{r}')$ can be considered as being 98 equal for large r'

$$U_A(r') = - \frac{e^2}{r'} \quad (5.3)$$

as a result of screening.

Then we have, according to formula (2.9)

$$\begin{aligned} i\hbar \dot{a}_0 &= - \frac{e^2 z^3}{\pi a^3} \int e^{-\frac{z}{a}(r+r')} \cdot \frac{d\tau}{r'} = - \frac{e^2 z}{a} (1 + zp) e^{-zp}; \\ w_0 &= \left(\frac{e^2}{\hbar v} \right)^2 \cdot 4z^2 \rho^2 \left[2K_1(z\rho) + \rho K_0(z\rho) \right]^2. \end{aligned} \quad (5.4)$$

We have arrived at the same formula which was used for the case of hydrogen. However, instead of ρ , we always have $z\rho$. Thus, we have in the final result

$$\sigma = \frac{\pi}{2z^2} \left(10.5 - \frac{1}{2} \ln \frac{E}{A} \right) = \frac{1}{U_i} \left(48 - 1.0 \lg \frac{E}{A} \right)^2. \quad (5.5)$$

This formula should be correct for atoms with one valence electron.

In the case when there are two valence electrons present we come to the case of helium, where both electrons reciprocally screen each other. We obtain analogously for atoms with two valence electrons

$$\sigma = \frac{\pi}{2z^2} \left(7 - 0.3 \ln \frac{E}{A} \right)^2. \quad (5.6)$$

We will mention however that the formula (5.5) also yields a fair result for helium. We obtain

$$\frac{\pi}{2} (7.9 - 0.37 \ln E)^2$$

instead of the more accurate

$$\frac{\pi}{2} (7.0 - 0.3 \ln E)^2.$$

6. COMPARISON WITH EXPERIMENTAL DATA

We will now examine to what degree the obtained results are confirmed by the experiment. Experimental results are absent in the case of atomic hydrogen. In the case of helium such results are available. Figure 3 gives the results obtained by Wolf. The interrupted line corresponds to the theoretical result from formula (2.13). From this graph it can be seen that the theory yields a result which exceeds somewhat the experimental data; however, it should be mentioned that /99 these data themselves are quite inaccurate and, as was shown by Sena, they require certain corrections.

The decrease in the cross section with energy also takes place somewhat faster than was predicted by the theory. The dot and dash line in Fig. 3 pertains to the evaluation which was made by Sena in his book,

$$\sigma = \frac{\pi}{2} \left(\frac{4e}{U_1} \right)^2. \quad (6.1)$$

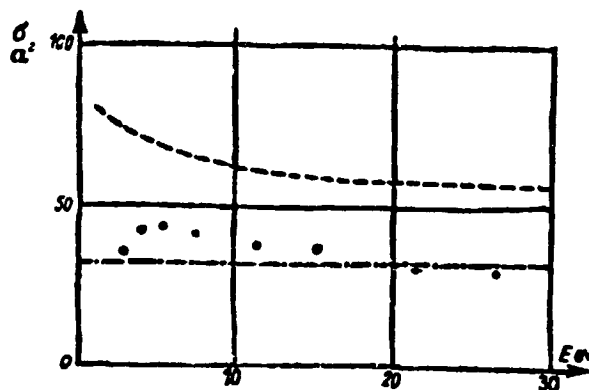


Fig. 3

However, this evaluation was made under assumptions which deliberately decreased the effective cross section.

In addition, it is possible to compare the general formula (5.5) for any given element with the experiment. The theoretical curve and the experimental points are given in Fig. 4.

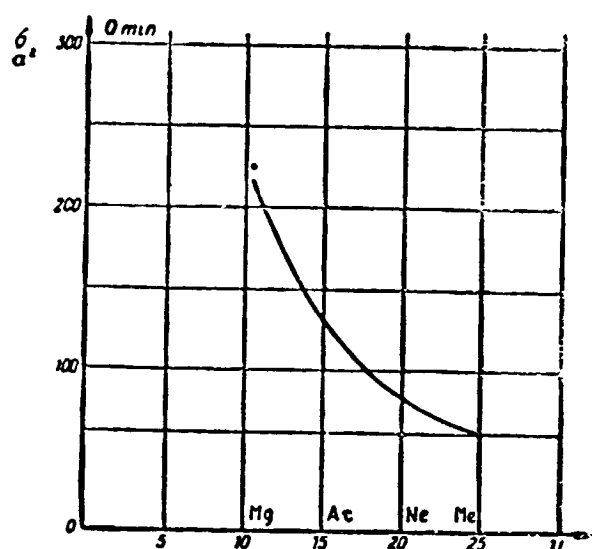


Fig. 4

Once again, the results in the majority of cases are somewhat lower than those given by the theory, with the exception of mercury. We will mention that the evaluation (6.1) of the dependence of the charge exchange cross section on the ionizing potential satisfies the experimental data much better, in spite of the fact that the conclusions are very loose and elementary.

The difference between the result which was obtained here and the result of an evaluation for elements with a low ionization potential, for instance in the case of potassium ($U_i = 4.3$ ev), will appear particularly marked. Measurement of the effective section of charge exchange for this case should serve in part as proof of the theory.

CONCLUSION

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In this manner we have calculated the complete cross section of a resonance charge exchange in the cases of hydrogen and helium, with the presumption that nuclei are in essence classical particles, and we have obtained formulae for the calculation of a differential effective cross section.

In addition we have obtained an approximate expression for the cross section of a resonance charge exchange in a general case. Further an evaluation of the applicability of the method was conducted and we have also evaluated how accurate a resonance level should be in order for the effective cross section to reach values which are common for a resonance charge exchange.

A comparison of the obtained results with the experiments yielded a satisfactory agreement.

The results proved to be applicable for the velocities of ions which are present in a plasma of a gas discharge.

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